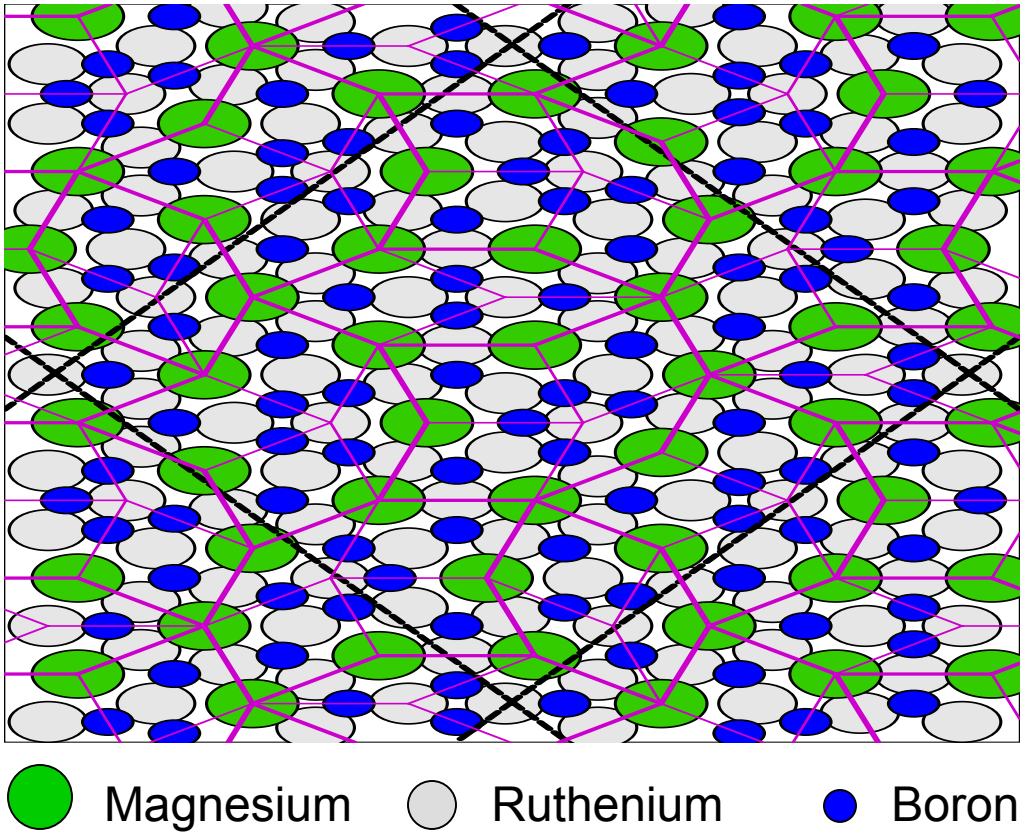
First-Principles Prediction of a Decagonal Quasicrystal

Predicting the structure and formation of metal alloys is crucial for achieving the goal of “Materials by Design”. Highly accurate methods for first-principles total energy calculation now allow the quantitative assessment of stable and metastable alloy phase diagrams. We have applied these methods to the study of previously unexplored alloy systems and to predict previously unkown structures.

Quasicrystals are materials whose structures contain crystallographically forbidden symmetries, such as pentagons. The figure at right shows a predicted B-Mg-Ru quasicrystal structure. This alloy is chemically and structurally unlike any previously known quasicrystal.



(Widom, DMR-0111198)